

Corrigé de l'exercice 4 - Série 4

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Ensemble grand canonique

la fonction de partition est donnée par:

$$Z_G = \text{Tr} e^{\beta(H - \mu N)} \quad \mu = \text{potentiel chimique}$$

$$= \text{Tr} e^{\tilde{\mu} N} e^{-\beta H} \quad \text{avec } \tilde{\mu} = \beta \mu$$

$$\Rightarrow Z_G = \sum_{N=0}^{\infty} e^{\tilde{\mu} N} \text{Tr} e^{-\beta H}$$

ona: $\text{Tr} e^{-\beta H} = Z(\beta, N)$ est la fonction de partition canonique à la température T fixe (β fixe) et pour le nombre de particules N .

$$\Rightarrow Z_G = \sum_{N=0}^{\infty} e^{\tilde{\mu} N} Z(\beta, N)$$

or la fonction de partition canonique est déjà calculée à l'exercice 3:

$$Z(\beta, N) = \frac{V^N \left(\frac{2\pi m}{\beta} \right)^{3N/2}}{N! h^{3N}}$$

$$\Rightarrow Z_G = \sum_{N=0}^{\infty} \frac{1}{N!} \left[\frac{e^{\tilde{\mu}} V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{h^3} \right]^N ; \text{ or } \sum_{n=0}^{\infty} \frac{x^n}{n!} = e^x$$

$$\Rightarrow Z_G = \exp \left\{ \frac{e^{\tilde{\mu}} V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{h^3} \right\}$$

$$\Rightarrow \log Z_G = \frac{e^{\tilde{\mu}} V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{h^3}$$

a) Energie moyenne: $\langle H \rangle = - \frac{\partial \log Z_G}{\partial \beta} \Big|_{\tilde{\mu}} = \frac{3 e^{\tilde{\mu}} V (2\pi m)^{3/2}}{2 h^3} \beta^{-5/2}$

b) Nombre moyen de particules:

$$\langle \tilde{N} \rangle = N = \frac{\partial \log Z_G}{\partial \tilde{\mu}} \Big|_{\beta} = \frac{e^{\tilde{\mu}} V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{h^3} = \log Z_G$$

on remarque que $E/N = \frac{3}{2} \frac{\beta^{-5/2}}{\beta^{-3/2}} = \frac{3}{2} \beta^{-1} = \frac{3}{2} kT \Rightarrow \boxed{E = \frac{3}{2} N kT}$

c) fonction de corrélation entre l'énergie et le nombre de particules:

$$G = \langle H \tilde{N} \rangle - \langle H \rangle \langle \tilde{N} \rangle = - \frac{\partial \log Z_G}{\partial \beta \partial \tilde{\mu}} = - \frac{\partial}{\partial \beta} \left[\frac{\partial \log Z_G}{\partial \tilde{\mu}} \right] = - \frac{\partial}{\partial \beta} (N) = 0$$

or $N = \log Z_G \Rightarrow G = - \frac{\partial \log Z_G}{\partial \beta} = E = \frac{3}{2} N kT$

d) fluctuations de l'énergie:

$$\langle H^2 \rangle - \langle H \rangle^2 = \frac{\partial^2 \log Z_G}{\partial \beta^2} = \frac{\partial}{\partial \beta} \left[-\frac{\partial \log Z_G}{\partial \beta} \right] = -\frac{\partial E}{\partial \beta} = \frac{3}{2} \frac{N}{\beta^2} = \frac{3}{2} N k^2 T^2$$

fluctuations du nombre de particules:

$$\langle \tilde{N}^2 \rangle - \langle \tilde{N} \rangle^2 = \frac{\partial^2 \log Z_G}{\partial \tilde{\mu}^2} = \frac{\partial}{\partial \tilde{\mu}} \left(\frac{\partial \log Z_G}{\partial \tilde{\mu}} \right) = \frac{\partial N}{\partial \tilde{\mu}} = \frac{e^{\tilde{\mu}} \cdot V \left(\frac{2\pi m}{\beta} \right)^{3/2}}{h^3} = N$$

e) Chaleur spécifique:

$$C_V = \frac{\partial E}{\partial T}; E = \frac{3}{2} N k T \Rightarrow C_V = \frac{3}{2} N k$$

f) le ^{grand} potentiel:

$$\Omega = -kT \log Z_G = -kT e^{\tilde{\mu}} \frac{V}{h^3} \left(\frac{2\pi m}{\beta} \right)^{3/2}$$

$$\Rightarrow \Omega = -e^{\tilde{\mu}} \frac{V}{h^3} (2\pi m)^{3/2} \beta^{-5/2}$$

g) Entropie: $S = k \log Z_G + \frac{E}{T} - \frac{\mu N}{T}$

on a $E = \frac{3}{2} N k T \Rightarrow \frac{E}{T} = \frac{3}{2} N k$ et on a: $\log Z_G = N$

$$S = N k + \frac{3}{2} N k - \frac{\mu N}{T}$$

$$\Rightarrow S = \frac{5}{2} N k - \frac{\mu N}{T}$$

h) pression:

on a $\Omega = E - TS - \mu N$

$$d\Omega = dE - TdS - SdT - \mu dN - Nd\mu$$

avec $dE = TdS - pdV$

$$\Rightarrow d\Omega = -SdT - pdV - Nd\mu$$

$$\Rightarrow P = -\left(\frac{\partial \Omega}{\partial V} \right)_{T, \mu}$$

$$\Rightarrow P = \frac{e^{\tilde{\mu}}}{h^3} (2\pi m)^{3/2} \beta^{5/2}$$

on a: $PV = \frac{e^{\tilde{\mu}} \cdot V (2\pi m)^{3/2} \beta^{5/2}}{h^3} = \underbrace{\frac{e^{\tilde{\mu}} \cdot V (2\pi m)^{3/2}}{h^3}}_N \cdot \beta^{-1} = N k T$

$$\Rightarrow \underline{PV = N k T} \quad \text{c'est l'équation d'état du gaz parfait.}$$